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DEVELOPMENT ARTICLE

The case in case-based design of educational software: A methodological interrogation

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Abstract This research assessed the value of case study methodology in the design of an educational computer simulation. Three sources of knowledge were compared to assess the value of case study: practitioner and programmer knowledge, disciplinary knowledge, and knowledge obtained from a case study of teacher practice. A retrospective analysis revealed that the case study was the source of 16 out of 23 design decisions and therefore was the most significant influence on the design of the simulation. The case study was particularly effective in sensitizing the design team to the classroom context, identifying common and uncommon teacher practices, revealing unexpected dimensions of interactions in the classroom, and generating constructive changes to the design of the simulation. Case studies can significantly enrich the design of educational software and are a promising methodological choice for design teams.

Keywords Software design · Computer simulation · Case study

Case study is rapidly becoming one of the most common forms of social science research (Stake, 2005; Yin, 2005). Because of the increasing use of case study in this regard, the focus of the present research was to inquire about the utility of case study methodology for informing the design of educational software. The method used to determine the utility of case study for informing educational software is a retrospective analysis of archived records and

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technical reports from a software design project. The major outcomes of this analysis are the delineation of a case-based design process, an assessment of the utility of case study for informing the design of educational software, and methodological considerations for employing case study to design educational software.

Background

The educational software in this study is a computer simulation to support students' understanding of unobservable phenomena in chemistry, such as interactions at the molecular level. Chemistry teachers and researchers have noticed that their students have difficulty conceptualizing chemistry at a molecular level (Coll & Taylor, 2001; Piquette & Heikkinen, 2005; Teichert & Stacy, 2002), in part because of the abstract nature of molecular interactions and the difficulties students have with managing a number of variables and seeing the effects of change. To produce a simulation that addresses this challenge, an interdisciplinary team of two lead chemistry teachers, three education researchers, four computer scientists with specializations in human-computer interaction, and a chemistry content expert, undertook the design, implementation, and testing of a novel computer simulation. The team, called the technology-enhanced model-based science or TEMBS team, conducted a three-month case study of teacher practice prior to the implementation of a prototype simulation in two high school chemistry classrooms. Once completing the project, the author who was a member of the team, sought to evaluate the utility of case study on the conceptual design of the software.

In the next section, the implications of case study on the design of educational software are suggested, and the potential significance of case study for the TEMBS project is considered.

Case study and potential implications for design

According to Stake, case study is the study of the particularity and complexity of a single, functioning, and bounded system (Stake, 1995, 2005, 2006). Case studies aim to give the reader a sense of being present, through a highly detailed analysis of "an instance in action" (MacDonald & Walker, 1977). Patton (1990) suggests that case studies are valuable in creating deep understanding of particular people, problems, or situations, in comprehensive ways. From an analysis of a single case, one can identify and describe basic phenomena and uncover new relationships and new perspectives on a topic (Merriam, 1988). According to Rueschemeyer (2003), another advantage of case study is that it permits a much more direct and frequently interplay between theory and data and allows for a closer matching of conceptual intent and empirical evidence than even exceptional quantitative research. At a

theoretical level, the power of case studies is in the ability to reveal the properties of the class to which the instance being studied belongs (Guba & Lincoln, 1981), produce new typologies (George & Bennett, 2005), provide the basis for subsequent theory-development (Kenny & Grotelueschen, 1984), and test and generate hypotheses (Flyvbjerg, 2001).

How case study is defined and conducted varies in the literature; however, certain properties are evident in a prototypical case study. The depth of study generally requires the study of a smaller sample size (Gomm, Hammersley, & Foster, 2000) than does survey research. Case studies yield highly descriptive accounts of a specific temporal and spatial boundary (Merriam, 1988) and uncover interactions of 'inseparable variables' that are elements of the phenomena being studied (Yin, 2003). As such, case study is appropriate for how and why research questions. Also, case study is suitable for research in complex settings where there is little control over behavior, organization, or events (Anderson, Crabtree, Steele, & McDaniel, 2005; Yin, 2003), because it advances the concept that natural complex settings cannot be reduced to a simple cause–effect relationship. Yin further argues that the use of multiple data sources allows for the development of converging lines of inquiry (or triangulation), providing a conclusion about a complex bounded setting that is likely to be much more convincing and accurate than survey research. In addition, case studies can generate working hypotheses based on what is uncovered or constructed during data collection in the case study (Eckstein, 2000; Lincoln & Guba, 2000). And finally, case studies are extendable in the sense that findings of a case study can enrich and potentially transform a reader's understanding of a phenomenon (Donmoyer, 1990).

Table 1 delineates the properties of a prototypical case and further suggests implications of case study on the design of educational software and the TEMBS project.

Overall, the properties of case study, such as the study of interactions in natural complex settings, use of multiple data sources, development of working hypotheses during data collection and analysis, and potential extendability of the findings of the case beyond the case itself, are amenable to the design of educational software and, in particular, aligned with the goals of the TEMBS design team. Because of this potential significance of case study, the TEMBS team utilized case study in their design process.

The next two sections detail how case study was embedded into a larger software design process and compares a process based on case study with design experimentation and participatory design.

A case-based design process

Case-based design includes case studies in the iterative and incremental development of educational software. In the TEMBS project, case-based design of the computer simulation involved the formation of an interdisciplinary design team (including the end-user, the teacher), identification of

Table 1 Properties of a prototypical case study and implications for the design of educational software and the TEMBS project

Properties	Design of educational software	TEMBS Project
In-depth study	Case study can reveal: educational problems, teacher expectations, school constraints, student interactions, conceptual challenges, and the potential for technology.	Case study allowed the TEMBS team to uncover and probe what students find conceptually challenging.
Bounded	Case study helps the researcher circumscribe the case according to existing temporal and spatial boundaries of the classroom.	The team wanted to develop rich hypotheses about the way a computer simulation could support students while they studied a conceptually challenging topic.
Focus on interactions	Many variables are at work in the success and viability of a computer technology (e.g., interactions between the technology and the user).	The team studied how students and teachers normally worked together to understand the ways interaction with a simulation could potentially foster student achievement.
Natural complex settings	Case study permits analysis of classrooms or informal educational environments, e.g., homes and centers.	The team studied a complex classroom environment to understand how a computer simulation could be embedded in existing instructional routines and practices.
Multiple data sources	Case study promotes the analysis of multiple forms of data to strengthen claims made about the software.	To produce a simulation that considers classroom dynamics, the team collected detailed observational data of classroom interactions, interviews with the teacher, and tests measuring student understanding.
Working hypotheses	Case study means researchers can remain open to serendipitous findings that might shape the direction of hypotheses.	The team wished to remain open to serendipitous findings about the classroom, as these findings might suggest new ways to configure the simulation.
Extendability	Case study presents concepts for how findings about one classroom studied can be extended to other classrooms.	The team wanted to extend the findings beyond the chemistry classroom studied so that other chemistry teachers would consider using the software.

team goals, identification of a pedagogical theory, a case study, a conceptual design of a simulation, creation of a prototype, field testing, and iterations to refine the computer simulation.

The case-based design process had 5 sequential phases as depicted in Fig. 1. Phases 1 and 2 were for planning, phases 3 and 4 were for development, and phase 5 was for testing of the software. This process, although bearing similarities to other design software development processes, is distinguishable by its inclusion of case study to inform phases 2 and 4.

Each of the five phases is elaborated below in the context of the TEMBS project.

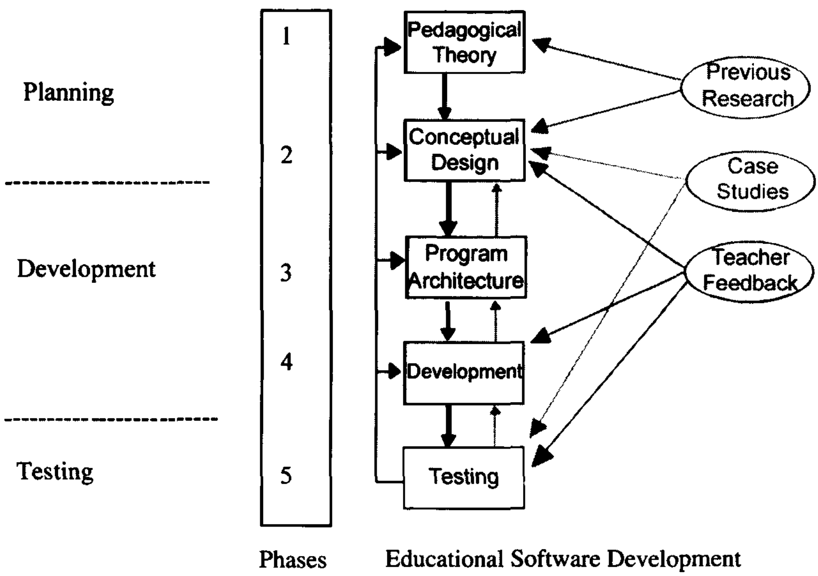

Fig. 1 Phases of a case-based design process of educational software

Phase 1: Pedagogical theory

After an interdisciplinary design team was assembled and broad goals for the project identified, the team read previous research on pedagogical theory over a four-month period in preparation for phase 2, conceptual design. A literature review on goal-based scenarios, metacognition, learning by design, complex systems, computer-supported collaborative learning (CSCL), embodied learning, and model-based teaching and learning (MBTL), was conducted by all members of the TEMBS team to identify a coherent pedagogical theory that could serve as a theoretical framework for the project. MBTL was selected for this project because the theory explicitly provides instructional guidance on helping students to develop mental models of unobservable phenomena, such as molecular structures.

Phase 2: Conceptual design

As depicted in Fig. 1, phase 2 was informed by the MBTL pedagogical theory, feedback from the teacher (who was a member of the design team), programmer knowledge, and a case study of teacher practice in a chemistry classroom. A brief summary of the case study is presented in the section, A Brief Case Summary of Teacher Practice in a Chemistry Class.

Phase 3: Program architecture

After the conceptual design of the simulation was developed, the computer architecture was constructed by the programmers who were members of the

TEMBS design team. Phase 3 also involved several meetings with the entire design team over a three-month period. The team met to discuss the congruence between the conceptual design developed in phase 2 and the program architecture of phase 3.

Phase 4: Development

Members of the TEMBS team with expertise in computer programming developed a prototype of a working simulation. Simulation prototypes were evaluated by all members of the team, including the teacher, for their congruence with the conceptual design. This phase required three months.

Phase 5: Testing

Testing of the simulation prototype occurred in four high school chemistry classrooms with feedback from the teacher and students. In two classrooms, quasi-experimental research was conducted. In the other two classrooms, a case study was conducted. The case study in the testing phase is not the focus of this paper, but the author mentions it to show that case study can also be utilized in the testing phase of design.

Before summarizing the case of teacher practice in a chemistry class, it is useful to compare the case-based design process with design experiments and participatory design.

A comparison of the case-based design process with design experiments and participatory design

The case-based design process contains several phases that are similar to traditional educational technology design research and basic principles of participatory design. Design research can be defined as the intentional design of objects (such as educational technologies) along with empirical research and theorizing about what occurs in authentic contexts in which the designed objects are used (Bell, 2004). Designs of educational technologies are implemented with a hypothesized learning process of the user in mind. If the hypothesis is refuted from testing, alternative hypotheses can be generated and tested. This leads to an iterative design process, in which the intended outcome is an explanatory framework that specifies expectations, such as expected interactions with the technology and how they might contribute to particular learning outcomes (Sandoval & Reiser, 1998). These expectations become the focus of investigation during the next cycle of inquiry (Cobb, Confrey, diSessa, Lehrer, & Schauble, 2003). Collins (1992) provided the following example of a first step in a hypothetical educational technology design research sequence:

> Our first step would be to observe a number of teachers and to choose [those] who are interested in trying out technology to teach students ... we would help the teacher design her own unit...using these various technologies, one that is carefully crafted to fit with her normal teaching (p. 19).

Edelson (2002) further delineated a design research process as a set of decisions on the design procedure with a team of experts, an analysis of some problem or needs assessment, and a design solution (essentially an effort to address the perceived problem or need). Edelson described the first phase as involving a review of the literature, a set of classroom observations, and a rapid prototyping of a tool. This phase was iterative in that it included a repeated refinement of the curriculum and software. The next phase occurred when students used the software and problem solutions to further refine the software and curricula. According to Edelson (2002), the potential outcomes of design research are lessons learned to create a successful product, and the generation of new domain theories, design frameworks (design principles), and/or design methodologies. In a case-based design process, the design procedure phase is similar to what Edelson described, except instead of a set of extended classroom observations, a formal case study is conducted. For the TEMBS project, a case study of teacher practice in a chemistry classroom was conducted.

Participatory design is a set of principles that embody user participation in the full process of design, not just the consumption of it. Participation of users in the design process blurs the boundaries between users and designers. In other words, the former end-users become co-designers of their learning environment. For educational software, this usually means involving teachers or students in the design process (Underwood, Hoadley, Digiano, Stohl, & Hollebrands, 2003), although it can also involve teachers as researchers. Principles of participatory design include mutual learning between the user and designer, application of design tools familiar to users, envisionment of future work situations, and analyses in the practice of the user (Chin, Rosson, & Carroll, 1997). The principles of participatory design are complementary to the case-based design process where the end-user, the teacher, is a co-designer of the simulation and provides feedback on the computer simulation prototype. As well, in a case-based design process, the analysis occurs in the context of the practice of the user, in this case, the classroom.

The next section briefly highlights a case study of teacher practice in a chemistry 12 classroom before the simulation was embedded in this context.

A brief case summary of teacher practice in a chemistry class

Although the focus of the paper is on the utility of case study for the design of software, the author includes a brief summary of the actual case study conducted for the TEMBS project as an example of the kinds of data that can be collected and major lessons learned from the full case study. Case selection,

context, and unit of analysis are included as subsections of the summary because they are unique methodological considerations of case study research. Other information about this particular case study, such as data coding issues, samples of instruments and student test scores, were not included in the summary for brevity but are available in the full case study report (Khan, 2004).

Case selection

A chemistry teacher was selected for this case study because he identified several learning challenges that were significant barriers to student success and representative of difficulties that chemistry students had with the subject material. He did not utilize digital technology in his teaching approach to chemistry, and because the design team wished to study how a computer simulation might enhance student understanding in chemistry, it was believed the effects might be more observable in environments where this technology was not used.

Context

The context of the case was a public grade 7–12 school with an enrolment of 910 students. The chemistry teacher taught two chemistry 12 classes ($n = 46$). Class A had 23 students (16 males, 7 females), and class B had 23 students (10 males, 13 females). Both classes were studying and reviewing Le Châtelier's Principle. This principle was identified by the teacher as the most challenging concept for chemistry students to learn and became the context for TEMBS software development.

Unit of analysis

The unit of analysis was the teacher's modeling practices. A teacher's modeling practice was operationalized as observable verbal or written teacher actions that fostered model-based learning in the classroom. Teacher's practices were encoded according to a classroom observation rubric. The decision was made to focus data collection on the teacher's practices because this would allow the TEMBS team to characterize common teaching approaches and identify how a computer simulation could enhance chemistry instruction moreso than a holistic analysis of classroom or school dynamics.

Multiple data sources

An interview with the teacher was conducted to identify his educational goals for students before the Le Châtelier unit commenced. All of the classes in the

Le Châtelier unit were subsequently observed by TEMBS researchers, totaling 375 min of observation. Classroom observation data consisted of field notes and video recordings. For each lesson observed, an observation rubric was filled in to record the frequency of 39 possible teacher and student actions based on MBTL theory (Khan, 2004). Other data collected included student handouts.

Data analysis

Multiple sources of data were analyzed for converging themes regarding teaching approaches.

Teacher goals

In the interview, the teacher stated that he wanted students to cover the curriculum, hone students' thinking skills, and ask more questions. From his experience of having taught this unit 29 times, he suggested that students' conceptual problems in chemistry came from difficulties with managing a number of variables and seeing effects of change. For example, regarding a chemical reaction with ammonia, he stated:

> The problem with the process is that there are many variable involved in the process (it gives heat, wants to break down). I feel that they [students] have difficulty grasping that there are many variables involved and that in changing one, it has a ripple effect on many other things... Students have difficulty seeing all the steps involved.

In summary, the teacher's goal was to help students improve their understanding of chemistry and overcome these conceptual difficulties.

General approach to instruction

As observed, a typical lesson in this unit began by taking up homework from the previous class or reviewing questions from the booklet. The teacher then introduced new concepts or theories from Le Châtelier's Principle, posed a question from a standardized assessment, and concluded with a lab. The next lesson would then involve take taking up homework questions on the board. The teacher stopped to review areas of student difficulty but he rarely had time to discuss Le Châtelier's Principle with students after the class.

Specific characteristics of instruction

In an assessment of the teacher's classroom delivery methods, it was found that he engaged in lecture discussion the most-about 30% of the time. Almost half of the class time was spent in either prepared lecture or lecture/discussion, and less than 14% of the time in doing hands-on activities either individually or in groups, or doing individual activities. The most frequently employed teacher actions were (starting with the highest frequency): quantitative

problem solving, accessing prior knowledge, finding analogies in chemistry, and offering explanations of conceptual models. Students were observed in more than three lessons: quantitative problem solving (answering the teacher's question), providing explanations of conceptual models, making comparisons, and evaluating their models of molecular structures in chemistry. Neither the teacher nor the students were observed using computers in class.

Summary

This summary highlights how several methodological considerations of case study—case selection, context, unit of analysis, and multiple data sources—were actualized in the TEMBS project. The full case study of the teacher's practice revealed a number of characteristics of the teachers' instructional approach and subsequently, students' learning experiences.

A. Students had:

1. particular challenges in grasping the multi-stage process of chemical reactions,
2. difficulty seeing the ripple effects of stressors on the system, and
3. problems seeing how equilibrium can be restored after a stress is applied.

B. The teacher:

1. taught predominantly in lecture mode, delivering content,
2. attempted to access students' prior knowledge before teaching a new concept,
3. provided students with regular feedback,
4. utilized analogy in his teaching to convey challenging concepts about equilibria,
5. employed examples from industry, and
6. did not use computers or simulations in his class.

C. Students were observed in class:

1. doing quantitative problem solving,
2. providing explanations of conceptual models, and
3. evaluating instructional models chemistry.

D. Students were not observed:

1. comparing molecular models,
2. isolating components or factors of molecular models,
3. making predictions to generate models,
4. analyzing graphs, or
5. expressing modifications to molecular models.

Thus, what was learned of teacher practice was that the teacher employed several strategies to promote understanding of chemistry at a molecular level, but other strategies were absent, such as asking students to compare molecular models and use computers.

The focus of the present research is on the utility of case study methodology for informing the design of educational software. The case summary provided in this section is intended to illustrate the kinds of findings that can emerge from a case study. The next sections proceed with an evaluation of the utility of case study for informing educational software, drawing upon this example.

Methods

The method used to evaluate the utility of case study for informing educational software is a retrospective analysis of archived records and technical reports from a software design project. A retrospective analysis of archived records was conducted to inquire about the utility of case study for the design of the TEMBS simulation. These records included:

1. a completed case study that included: a literature review on student challenges in chemistry and a review of existing software on the topic, methods, analysis of classroom data, and an extensive discussion of lessons learned from the case;
2. archived bimonthly and weekly TEMBS meeting minutes for a one-year period;
3. all e-mail communications with the members of the TEMBS team;
4. all drawings of computer simulation prototypes, and
5. two technical reports on the architecture of the simulation (Khan et al., 2005).

The above documents formed the basis for an assessment of the utility of case study for the design of software.

Firstly, the assessment was conducted by listing all of the design features in the simulation and locating the source of these major conceptual decisions. For example, the TEMBS simulation incorporated a dynamic analogy of chemical equilibrium using a depiction of a scale. The source of the decision to utilize analogy was traced to the case study, where it was observed that the use of analogy was identified as one of the top 5 instructional strategies employed by the teacher in the Le Châtelier unit.

Secondly, the design decisions were coded as being from: (a) disciplinary knowledge (knowledge from literature review), (b) practitioner knowledge (programmer knowledge, intuitions or hunches from programmers, and chemistry teacher's feedback), or c) lessons learned from the case study. These knowledge sources were not mutually exclusive; that is, a conceptual design decision may have come from more than one of the above knowledge sources. A second examination of the data took this into account. For example, the decision to create a nanoscale view in the simulation came from

both case study and disciplinary knowledge (in the form of a literature review of MBTL theory). The case study revealed that students were not comparing molecular models, and the literature review suggested that students learn by evaluating and modifying their models of unobservable phenomena such as molecular structures. By introducing a nanoscale view in the simulation, a working hypothesis was developed that students will visualize animated molecules and that visualization of molecules will afford students the opportunity to compare and evaluate models at the molecular level.

Thirdly, a location matrix was created to pinpoint empirically from the data corpus the number of times case study was the source of the design decisions for the software. This was accomplished by locating the intersection between the knowledge source (on the x-axis) and the design feature of the software (on the y-axis). Appendices A–C provide an elaborated matrix with the addition of a column on working hypotheses.

Finally, case study methodology was evaluated for its capacity to fulfill five criteria.[1] These criteria are important to the case-based design process because they address the ways case study could impact the design of software.

1. Extract specific challenges with particular concepts;
2. characterize teaching and students' responses to teaching;
3. prepare for the introduction and integration of new software into a classroom environment;
4. produce viable design options for the software, and
5. generate working hypotheses about how the design of the software addresses students' conceptual challenges.

Results

In phases 1 and 2 of the case-based design process, the TEMBS team planned the conceptual design of the software. Results of how disciplinary knowledge, case study knowledge, and practitioner knowledge influenced the conceptual design of the simulation are presented using two illustrative examples from each source.

Disciplinary knowledge

Phase 1 of the case-based design process involved identifying a pedagogical theory. The chief source of information on pedagogical theories came from disciplinary knowledge. For example, in a review of educational literature on model-based teaching and learning, the TEMBS team found that building, critiquing, and transforming mental models of the way the world works can be linked with positive gains in student understanding. For this reason, the TEMBS team decided to incorporate a dynamic simulated model of molecular

[1] These criteria were reviewed by an expert in the field of case study who was not affiliated with the TEMBS project.

structures in the simulation. The working hypothesis was that a simulation that included animated models of molecules will help students to develop their mental models of molecular structures by: (a) manipulating variables associated with the simulated model to extremes, (b) creating what-if scenarios with the simulated model, and (c) visualizing animated representations of unobservable phenomena via the simulated model.

In a second example of how disciplinary knowledge was the source of a conceptual design decision, the TEMBS team found that viewing several representations of a chemical reaction (e.g., macromolecular, symbolic, molecular) has potential to promote deep learning in chemistry (Kozma, 2000). Therefore, the team decided to create three different representations of chemistry that were viewable on the interface: chemistry at the symbolic level (formula bar), chemistry at the macromolecular level (graphical representation of concentrations of reactants and products over time), and a nanoscale view (animation of moving molecular spheres representing each chemical). The TEMBS team hypothesized that providing students with several representations of chemistry will foster conceptual links among the bulk chemical reaction, individual molecules during the reaction, and the symbolic language of chemistry. Appendix A is an extended table that shows the extent to which disciplinary knowledge influenced the conceptual design of the simulation and the creation of working hypotheses regarding the effectiveness of the simulation.

Case study knowledge

In Phase 2, the TEMBS team completed planning the design of the simulation. The conceptual design of the simulation was informed in part by a case study of teacher practice. For example, the case study revealed that the teacher used verbal analogies as one of the top five surveyed teaching strategies. The TEMBS team decided to create a dynamic analogy to a chemical reaction to: (a) bridge the use of common instructional strategies in the classroom with the simulation, and (b) animate static analogies presented by the teacher. The team conceived of an analogy of chemical equilibrium in the form of a tilting weigh scale. A working hypothesis of the TEMBS team was that a dynamic analogy of the chemical reaction to a simulated weigh scale will enhance instruction by the teacher. Furthermore, the team hypothesized that an explicit connection between the chemical reaction and the analogy, in which the analogy view was mapped to reaction parameters in the simulation, would be beneficial for students' construction of a mental model of chemical equilibrium.

In a second example of how case study influenced the conceptual design of the simulation, the case study revealed that students have trouble grasping the multi-stage process of chemical reactions. To help students recall and compare different phases of a chemical reaction, the TEMBS team designed time-stamping and roll-back features and incorporated them into the simulation's graph view. Time-stamping and roll-back meant that students can double

double-click on a point on the graph to rewind the reaction to a particular point, enabling replay of the reaction. These features were hypothesized to help students grasp the stages of the reaction. Appendix B is an extended table that further delineates all that was learned from the case study and how case study influenced the conceptual design of the simulation and the creation of working hypotheses regarding the effectiveness of the simulation.

Practitioner knowledge

The programmers' insights and feedback from the teacher (both considered practitioners and members of the design team) also contributed to the conceptual design of the simulation. For example, the teacher said during phase 2 of the case-based design process: "It would be valuable for students to see how a change in pressure, temperature, and concentration would be operable in the simulation for both gases and non-gases." Therefore, the TEMBS team included reactions that involved gases and non-gases. The programmers, however, stated that users sometimes engage in random clicking behaviors when playing online games or working with simulations: "Clickfests happen when users keep clicking buttons randomly to get to the next level or next step. Let's avoid that." To avoid clickfests, the team built in structure that would focus students' attention on questions related to the graph of the simulation. Direct questions were placed in a question box on the interface and the question would have to be answered before the simulation could proceed. Appendix C is an extended table that lists how practitioner knowledge influenced the conceptual design of the simulation.

A comparison of case study with disciplinary and practitioner knowledge

Table 2 displays the full spectrum of conceptual design decisions and pinpoints which knowledge source [disciplinary knowledge (DK), case study knowledge (CK), and/or practitioner knowledge (PK)] led to the design decision using a dot.

As displayed in Table 2, the case study resulted in the production of 16 out of 23 design features and concomitantly, the generation of 16 working hypotheses about how the design of the computer simulation addresses students' conceptual challenges (see Appendix B). Practitioner experience and literature reviews influenced 7 out of 23 design features in the simulation. Thus, the case study exceeded practitioner and disciplinary knowledge as the origin of decisions for the conceptual design of the software.

Discussion

The focus of this research was on evaluating the utility of case study for the planning of an educational software's conceptual design. This paper used the example of the TEMBS project, and the case study associated with it, to assess

Table 2 Comparison of three knowledge sources (KS) and their Influence on conceptual design

#	Conceptual design decisions	KS		
		DK	CK	PK
1	Incorporated dynamic models of molecular structures.	•		
2	Displayed an interactive graph, sliders, &nanoscale view.	•		
3	Full complexity of chemical equilibrium is presented at once, rather than the conditional release of the model.	•		
4	Three views were represented in the interface: 1) chemistry at the symbolic level (formula bar), 2) chemistry at the macro-molecular level (graphical representation of concentrations of reactants and products over time), and 3) a nanoscale view (animation of moving molecular spheres representing each chemical).	•		
5	A question box is created with limited feedback.		•	
6	The simulation is introduced when student construction and evaluation of models was taking place in the lesson.		•	
7	The simulation would not be a simulated chemistry lab, as it was not intended to replace the only hands-on activities in the class.			
8	The simulation presents an analogy of chemical equilibrium.			
9	The simulation will provide only essential background information about a particular chemical reaction.		•	
10	A familiar image to students, a tilting scale, is utilized as an analogy to equilibrium.		•	
11	Time-stamping and roll-back features are incorporated in the graph view.		•	
12	A central simulation engine synchronizes different views of the simulation.		•	
13	A prediction mechanism is built into the simulation. Students can make a prediction about what the graph will do next.		•	
14	A nanoscale view is built into the simulation.	•	•	
15	Sliders of: concentrations of chemicals, volume, and temperature are available to isolate and vary factors individually or together.		•	
16	Color-coding is included in the simulation.		•	
17	The scale analogy shows that forward and reverse reactions still occur at equilibrium, as chemicals continue to cross from one side of the scale to the other.		•	
18	Chemical equations are of industrial plant or everyday processes.		•	
19	The speed of molecules is modulated by temperature.			•
20	Students are able to pause a reaction and make predictions about it before the next phase of the reaction is revealed on the graph.			•
21	Graphs show that the concentration of each chemical changes with temperature changes.			•
22	The simulation contains choices of reactions.			•
23	Direct questions are asked in the question box.			•

the utility of case study for the conceptual design of a chemistry computer simulation. From a case study of teacher's practice in a chemistry classroom, the TEMBS design team was able to effectively:

- extract specific challenges students had with grasping the multi-stage process of chemical reactions;
- characterize the teaching approach as following a didactic instructional pattern that involved the use of analogies to explain difficult concepts;
- prepare for the integration of new software into a predominantly lecture and lecture-discussion oriented classroom environment,;
- produce 16 viable design options for the software, and
- generate an equal number of working hypotheses about how the design of the software addresses students' conceptual challenges.

For example, in-depth examination of teacher practice via case study revealed that the teacher frequently used analogies when describing difficult topics. Unlike analogies used in other software, the TEMBS simulation explicitly linked the functionality of the analogy to the chemical reaction. This stronger explicit connection between the reaction and the analogy is hypothesized as beneficial for visualization and generation of mental models.

The case study also revealed that students were not generating molecular models of chemical equilibria, although they were being asked to evaluate instructional models of chemistry. The TEMBS simulation afforded students the opportunity to enrich their conceptions of chemical equilibria by visualizing molecular models and providing a simulated mechanism for students to construct connections across various representations of chemistry. Students were also able to compare before and after changes to their models by replaying reactions, something impossible to achieve in a chemistry lab.

The case study further revealed that the teacher performed tasks such as providing content and feedback to students and, in the view of the design team, these tasks did not need to be replaced by the simulation. Rather, the TEMBS team designed the simulation to enhance model-based teaching and learning, augment practices already observed in the classroom, and support student activities that were not apparent during classroom instruction. As these examples illustrate, design teams can learn from the in-depth examination of a phenomenon that is case study and the insights case study reveals, such as students' conceptual challenges and characteristic teaching behaviors in the classroom. The influence of case study methodology on the novel conceptual design of the simulation was significant, and the majority of design decisions were based on the case study.

Conclusions

Case studies leverage a typical design process by: (a) sensitizing the design team to the classroom context, (b) identifying common and uncommon

teacher practices, (c) revealing unexpected dimensions of interactions in the classroom, and (d) generating constructive changes to the design of the software. Case-based design is an educational software design process that utilizes case study in both the planning and testing of educational software. An important consideration before engaging in case-based design is the time it takes to do a case study. In the TEMBS project, the case study took 3 months. The author argues, however, that this time was well spent, given the significant and constructive influence a case study had on the conceptual design of the TEMBS computer simulation. As a corollary, the author suggests a re-examination of the need for rapid prototyping in the educational software industry, especially in light of poor reports of the viability of educational software in classroom settings.

A second point regarding case-based design has to do with producing highly customized software, software that may be in danger of having little impact beyond the case context. The TEMBS team designed the software with the intention that it would be useful for the chemistry teacher of the case study and other chemistry teachers who are interested in new ways to teach equilibrium chemistry. Often times, if educational software gets tested with users in the classroom, the test occurs in one classroom, not all possible classrooms where the software could be integrated. Thus, the generalizability of findings from a single case was not a primary goal in the planning stage; however, subsequent applications of the software would test the working hypotheses generated from the case.

Positivist notions of generalizability have been largely abandoned or modified in social science and case study scholarship (Donmoyer, 1990; Guba & Lincoln; 1981; Schofield, 1990). Generalizations have been recognized as contextual, having half-lives (Cronbach, 1975) that required updating (even in experimental research): "It is far easier, and more epistemologically sound, simply to give up on the idea of generalization. If they are accepted, they should be as indeterminate, relative and time and context bound" (Lincoln & Guba, 2000, p. 32).

Instead of positivist notions of generalizability, new concepts involving comparison of cases have been applied to case study research to extend and amplify the effect of a single case beyond the case itself (Becker, 1990; Smaling, 2003; Yin, 2003). For example, Goetz and Le Compte (1984) recognized that the findings from case studies cannot be generalizable in a probabilistic sense, but that findings may still be relevant to other contexts. Comparability is a concept they proposed to address the issue of generalizability from a single case. Comparability is the degree to which the parts of a study are sufficiently well described and defined so that other researchers can use the results of the study as a basis for comparison. Translatability is a similar concept but refers to a clear description of one's theoretical stance and research techniques.

The concepts of comparability and translatability provide insights on how a case study of educational software in a bounded classroom context can be extended to learning environments that were not directly studied. To compare

one case with another, dimensions of the cases should be similar or belong to similar categories. For example, this case study revealed a conceptual challenge regarding the equilibrium concept for the chemistry students, a problem that is widespread as substantiated in the literature. It is therefore plausible that other chemistry students would encounter similar conceptual challenges. In addition, the instructional approach of the teacher could be considered somewhat traditional, and the classroom space was a traditional, non-technology enhanced environment for learning science. A similar instructional approach and classroom environment might be present in other settings. Similarities among chemistry students' conceptual difficulties, teaching approaches, and classroom space suggest that the findings from this case may be comparable and translatable to classroom contexts beyond the case studied. To the TEMBS team, the comparability and translatability of this case bodes well for producing a simulation that may be utilized in many chemistry classrooms with different teachers and students.

In summary, case studies can contribute towards, "fram[ing] the context which a given innovation has been shown to be effective, so that schools... have a sound basis for deciding which innovations to adopt" (Lesgold, 2003, p. 73). By elaborating on the classroom, the case has the potential to inform and enrich the development of educational software that is intended to support existing teacher practice, emphasize practices that are not evident in the classroom, and promote student learning. As such, case studies offer a promising methodological choice for educational software design teams.

Appendix A

Table A1 How disciplinary knowledge influenced the conceptual design of the simulation

Disciplinary Knowledge	Design decision for the TEMBS simulation	Working Hypothesis
Model-based teaching and learning involves building, critiquing, and transforming one's own mental models of the way the world works.	The TEMBS simulation incorporated dynamic models of molecular structures in the form of a molecular view.	A computer simulation will help students to develop their mental models of molecular structures by manipulating multiple variables to extremes, creating what-if scenarios, and visualizing animated representations of unobservable phenomena in science. Students can make an informed evaluation of their own mental models of how the reaction is proceeding and this is beneficial to learning (Khan, 2002).
Review of interactivity found in software for chemical equilibria: ChemEquilibria (Blauch, 2001), NetLogo (Wilensky, 1999), E-chem (Wu, Krajcik, & Soloway, 2001), Chemland (Vining, 2000).	Production of interactive: graph, sliders & nanoscale view.	Interactivity is beneficial to student learning because students can experiment with what if scenarios to test their hypotheses (Khan et al., 2005).
Model progression may not have an impact on learning (Quinn & Alessi, 1994; Alessi, 1995; Rieber & Parmley, 1995).	Full complexity of chemical equilibrium is presented at once, rather than the conditional release of additional variables or models.	Students will control variables as a function of their need to identify causes and effects in the system. Oversimplification of molecular models would reduce cognitive overload and in addition to control of variables, more easily identify cause and effect.
Viewing multiple representations (eg. macromolecular, symbolic, molecular) in chemistry has potential to promote learning (Kozma, 2000).	Three views of chemistry were represented in the TEMBS interface: chemistry at the symbolic level (formula bar); chemistry at the macromolecular level (graphical representation of concentrations of reactants and products over time), and a nanoscale view (animation of moving molecular spheres representing each chemical).	Providing students with multiple representations of chemistry will provide a data rich environment for students to make links between what is happening to the bulk reaction, what is happening to individual molecules during this reaction, and how this reaction is represented using the symbolic language of chemistry.

Appendix B

Table B1 How the case study influenced the conceptual design of the simulation

What was learned from the case study	Design decision for the simulation	Working Hypothesis
The teacher provides feedback for students.	Feedback was limited to correct or incorrect answers in the question box.	The simulation would be best embedded in the normal day to day activities of the chemistry unit, where small and large group discussion with the teacher was fostered.
The teacher's instructional approach had a general pattern.	The simulation should be introduced when student construction and evaluation of models is taking place.	The simulation affords students the opportunity to generate effect to cause models.
Hands-on activity is not evident as much as lecture.	The simulation is not intended to replace labs (the only hands-on activities in the class).	The simulation affords students with opportunities to visualize what is happening at a molecular level and manipulate variables in a chemical reaction.
Teacher use of analogy was identified as one of the top 5 teaching strategies used in this unit.	Simulation presents an analogy of chemical equilibrium in the form of a tilting scale.	A dynamic analogy of the chemical reaction to a scale will enhance instruction of the teacher.
		An explicit connection between the reaction and the analogy, where the analogy view is mapped to reaction parameters, is beneficial for students' construction of a mental model of chemical equilibrium.
Teacher teaches predominantly using a lecture &lecture/discussion format.	The simulation will provide only essential background information about a particular chemical reaction, since the teacher is delivering copious amounts of information in lecture.	The simulation will afford students with an opportunity to test, generate, and enrich their understanding of equilibrium.
Teacher asked students to access their prior knowledge.	A familiar image to students, a scale, is utilized in the simulation as an analogy to chemical equilibrium.	Students in chemistry labs have observed scale mechanics and daily life and this tacit knowledge can act as an initial trigger for students to compare their model of a chemical reaction to a familiar model of a scale.
Students have trouble grasping the multi-stage process of chemical reactions.	Time stamping and roll-back features are incorporated in the graph view. Students can double click on a point on the graph to 'rewind' the reaction to a particular point in time, enabling replay of the reaction.	Students will be able to recall and compare different phases of a chemical reaction with the assistance of the time-stamping and roll-back features in the graph view.

Table B1 continued

What was learned from the case study	Design decision for the simulation	Working Hypothesis
Lab activities reveal that students are required to coordinate chemical symbols with reactions.	A central simulation engine synchronizes 5 different views of the simulation.	Multiple simultaneously viewed information streams will provide students the opportunity to connect the macromolecular level with the molecular level of the chemical reaction.
Students were not observed making predictions to generate models.	A prediction mechanism is built into the simulation. Students can make a prediction about what the graph will do next. If the prediction option is enabled, students are asked questions via a text box about concentration changes. This question is given as a 4-point multiple-choice question that must be answered before the simulation can be run again.	The prediction mode supports this activity in the class. Students who make predictions reveal and test their mental models of reactions.
Students were not observed comparing molecular models.	A nanoscale view was built into the simulation.	Visualization of molecules affords students the opportunity to compare molecular models according to the changes they make to the variables in the reaction.
Students were not observed isolating components or factors of molecular models.	Sliders of: concentrations of chemicals participating in the reaction, volume and temperature are available for students to isolate and vary factors individually or together.	Students will be able to isolate factors responsible for changes to the chemical reaction using the sliders in a systematic fashion.
Students were not observed analyzing graphs.	A graph view was created for the simulation.	Graphs will afford students the opportunity to visualize and analyze how a chemical reaction proceeds over time and compare how individual concentrations change over time.
Students were not observed expressing modifications to molecular models.	Students can compare several representations of the reaction in the simulation: symbolic, molecular, scalar, and graph, all by concentration and by time.	Comparing representations of reactions will help students to modify their mental models of molecular structure and behavior.
Students had difficulty grasping that changing one variable has a ripple effect on many other aspects of a chemical reaction. The teacher also stated that students have difficulty seeing all the steps.	Color-coding was included in the simulation. Students can change variables in the simulation and then trace chemical changes in the graph and analogy views, as the chemicals are color coded across all views. The chemical engine synchronizes all views to the reaction.	Being able to trace how a chemical reaction proceeds at a macromolecular and molecular level with purposeful color coding will promote understanding of the variables involved in a chemical reaction and ripple effects on multiple variables when one variable is changed.

Table B1 continued

What was learned from the case study	Design decision for the simulation	Working Hypothesis
Teacher identified that students need to see how equilibrium can be restored after a stress is applied.	The scale analogy shows that forward and reverse reactions still occur at equilibrium, since chemicals continue to cross from one side of the *scale to the other*.	Students' visualization of chemical reactions using the scale analogy will help students understand how a stress applied on the chemical system can effect equilibrium and how *different parameters can influence* how equilibrium can be restored.
Teacher discusses chemical reactions that come from industrial plants or everyday processes.	Database of chemical equations available in the simulation come from industrial plants or everyday processes.	Reactions stored in the simulation are ones that fit into the current curriculum and extend students' understanding of industrial processes.

Appendix C

Table C1 How practitioners influenced the conceptual design of the simulation

What was learned from practitioners	Design decision for the simulation
Teacher feedback: "It would be helpful for a screen to show, for example, how the speed of the molecules change with a change in temperature".	The speed of molecules was modulated by temperature of the chemical reaction.
Teacher feedback: "I have found that demonstrations in class are more effective when students get a chance to predict what they are going to observe before seeing the result."	Students are able to pause a reaction and make predictions about it before the next phase of the reaction is revealed.
Teacher feedback: "Since Keq = concentration of products/concentration of reactions, students should be able to see how with only temperature changes, the ratio of products to reactants changes and therefore the value of Keq changes."	Confirmed that graphs show that the concentration of each chemical changes with changes to temperature.
Teacher feedback: "It would be valuable for students to see how a change in pressure, temperature, and concentration would be operable in the simulation for both gases and non-gases."	Simulation will have choices of reactions that will include gases and non-gases.
Programmer feedback: "Clickfests are when users keep clicking buttons randomly to get to the next level or next step. Let's avoid that."	Direct questions are asked in the question box. This built in structure may help students avoid "playing" with the simulation and guide inquiry and discovery. Secondly, if the prediction option is enabled, a question must be answered before the simulation can be run.

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